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ON THE MATHEMATICAL THEORY OF DEFLAGRATIONS AND DETONATIONS

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ON THE MATHEMATICAL THEORY OF DEFLAGRATIONS AND DETONATIONS

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ON THE MATHEMATICAL THEORY OF DEFLAGRATIONS AND DETONATIONS

1. NavOrd Report 79-46 presents the results of an investigation carried out by Dr. K.O. Friedrichs of the Institute for Mathematics and Mechanics at New York Universtiy under Contract Noa(s) 7370, Bureau of Ordnance, Navy Department, to determine the propagation of reaction processes.

2. This report presents preliminary data and therefore does not constitute a final comprehensive study. Additional information and criticism by other agencies is invited.

3. The findings herein represent the interpretation of the author and are not necessarily the views of the Bureau of Ordnance. The Bureau of Ordnance liaison officers were Dr. R.J. Seeger and Dr. R.J. Finkelstein.

4. This report does not supersede any existing publication.

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Vice Admiral, U.S. Navy
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INTRODUCTION

The present investigation was carried out by Dr. K. O. Friedrichs of the Institute for Mathematics and Mechanics at New York University under Contract NOa(s)-7370, Bureau of Ordnance, Navy Department. It continues the work done for the Applied Mathematics Panel of the National Defense Research Committee in particular the Supplement, "Remarks on the Mathematical Theory of Detonation and Deflagration Waves in Gases," to the Manual on "Supersonic Flow and Shock Waves."

Thanks are due to Dr. Robert Finkelstein and Dr. James Savage for many critical comments and suggestions.

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On the Mathematical Theory of Deflagrations and Detonations

While the propagation of a shock wave is completely determined by the conservation laws, the boundary conditions of the problem, and the additional condition that the entropy increase in the process, the same is not true for the propagation of a detonation wave and of the flame front in an ordinary combustion process. More conditions must be added to the conservation laws in order to provide sufficient data for the unique determination of the propagation process. For detonations this necessity was recognized by Chapman and Jouguet when they introduced their famous hypothesis. For combustion processes this necessity was more or less tacitly assumed by Jouguet and others when they attacked the calculation of the flame speed by taking heat conduction into account without even trying to determine the flame speed from the conservation laws and boundary conditions alone.

It is natural to expect that the needed additional conditions could be derived from an investigation of the internal mechanism of the combustion or detonation process. Thus v. Neumann [1] has arrived at a justification of the Chapman-Jouguet hypothesis for detonations by taking into account that the chemical reaction takes place over a zone of finite width; his arguments are based on the assumption that a detonation is initiated by a shock. For combustion processes, which do not involve shocks, no unique determination can be achieved without taking heat conduction into account.

It is the intention of the present paper to offer a unified and more complete discussion of the question of determinacy for detonations and deflagrations.[1] In order to be able to point out the contrast between these two kinds of processes we shall treat both of them on the basis of the same assumptions: We shall take viscosity and heat conduction into account and assume a finite rate of chemical reaction. (Accordingly, we shall not postulate that a detonation process begins with a shock.) From the discussion of the internal mechanism of the detonation and deflagration process on this basis we shall obtain the desired additional conditions which make unique determination of the whole process possible by excluding certain detonation or deflagration processes which would be compatible with the conservation laws. In particular we shall find as a result that a detonation begins with a shock and that the Chapman-Jouguet hypothesis furnishes the correct additional condition provided that for a given value of the reaction rate the viscosity and the heat conductivity are sufficiently small. If, on the other hand, the reaction rate is very high, for given viscosity and heat conductivity, the detonation no longer begins with a shock; and if the reaction rate is excessively high, the Chapman-Jouguet hypothesis is no longer correct; (see Appendix II). The additional condition for deflagrations is such that it prescribes the flame speed dependent on heat conduction and reaction rate.

To fix the ideas we have considered the problem of determining the flow under the following circumstances: In an infinite tube a piston moves in a prescribed manner beginning at an initial time at an initial cross-section. At the same time a reaction process begins at the piston and travels into the quiet unburnt gas.

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[1] We propose to use the term deflagration for those combustion processes which take place in a very narrow zone of constant width and which therefore in good approximation can be described by a discontinuity. For detonation and deflagration processes we shall employ the common name "reaction process".

This problem includes the important case that the tube is closed at the initial cross-section; for, this case results when the piston remains at its original place. The case of an open end results when the piston is withdrawn with sufficiently large speed. Also the case is included that in a doubly infinite tube containing combustible and non-combustible gas, not separated by a piston, a reaction begins at the interface. One needs only force the piston to move in the same manner in which the initial cross-section would move anyhow if there were no piston.

Before describing the results in greater detail we formulate the basic assumption underlying our investigations viz. that the reaction process in question may approximately be considered as a sharp discontinuity. More precisely the assumption is that the "reaction zone," across which chemical composition, pressure, temperature, and velocity change is very narrow and of nearly constant width; (see Appendix I). By this we mean, firstly, that the space rates of change of the pertinent quantities over a section in the field of flow outside of the reaction zone are negligibly small when compared to the rates of change of the same quantities inside the reaction zone and, secondly, that the time rate of change of the width of the reaction zone is small when compared with the average speed with which the gases cross the reaction zone. This assumption appears to be justified only if the coefficients of viscosity and heat conduction are sufficiently small and the rate of reaction is sufficiently large. (We leave aside the question whether or not under these circumstances the assumption is always justified.) The pertinent quantities on both sides of the "reaction front" are then connected by the same well-known laws of conservation of mass, momentum, and energy that hold for the quantities at both sides of a discontinuity surface.

Next we give a brief account of the indeterminacies that one encounters when one tries to determine a flow involving a reaction discontinuity solely by using the conservation laws and the boundary conditions. To this end it is necessary to distinguish various types of reaction processes. Among the detonations there is, as is well known, a particular one, the "Chapman-Jouguet" detonation, which is singled out from others by the property that the flow of the burnt gas is sonic when observed from the reaction front. We have termed "strong" or "weak" a detonation if it involves a pressure rise greater or less than for a Chapman-Jouguet detonation.[1)] Similarly, we have termed "strong" or "weak" a deflagration if it involves a pressure drop greater or less than for a Chapman-Jouguet deflagration, which again is characterized by the condition that the flow burnt gas is sonic when observed from the reaction front. A constant volume detonation is the limiting case of a weak one, producing the least pressure rise (and the least temperature rise) among all detonations for the same explosive; a constant pressure deflagration is also the limiting case of a weak one, producing the least drop in density (and the greatest temperature rise) among all deflagrations.

We now consider the flow of gas in a half-finite tube resulting, as indicated before, when a reaction front starts to move from the finite end of the tube into the unburnt gas under the influence of a piston which moves in a prescribed manner. We then ask for the gas motions which are compatible with the conservation laws and the piston motion. Mathematically speaking, we ask for the solutions of the flow differential equations compatible with the transition conditions at the discontinuity front and with the boundary condition, which expresses that the gas adjacent to the piston has the same velocity as the piston. This problem will be referred to as the "external flow problem." The

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[1)] For the following see the Supplement [3] to the Manual on Supersonic Flow and Shock Waves [2] .

answer, explained in detail in an earlier report [3] is this:[1] Suppose the reaction process is a detonation; if then the piston moves in the same direction as the reaction front, and if the velocity u_P of the piston exceeds the gas velocity u_D which would be produced by a Chapman-Jouguet detonation, then there is just one flow involving a strong detonation in which the burnt gas has the prescribed piston velocity. If, however, the piston velocity u_P is less than u_D, adjustment of the velocity of the burnt gas to the piston velocity can always be achieved by a Chapman-Jouguet detonation followed by an appropriate rarefaction wave, but it can also be achieved by a set of weak detonations followed either by a shock or a rarefaction wave. Thus, in case $u_P < u_D$, the solution of the mathematical problem is not unique; there is a one-parametric set of solutions.

For deflagration processes the degree of indeterminacy is still higher. To any piston velocity u_P one has still the choice of a flame velocity arbitrary within certain limits[2] and can achieve adjustment of the gas velocity to the piston velocity by sending ahead of the flame a shock of appropriate strength. Again, there is a one-parametric set of solutions as long as the deflagration remains weak. If the resulting deflagrations become strong ones, the possibilities of adjustment become still greater and the set of solutions is two-parametric.

To express these determinacy statements in a simple form we introduce as "degree of under-determinacy" of the external flow problem the number t of conditions that must be imposed on the data of the flow problem in order to make the solution unique. Summarizing we then have:

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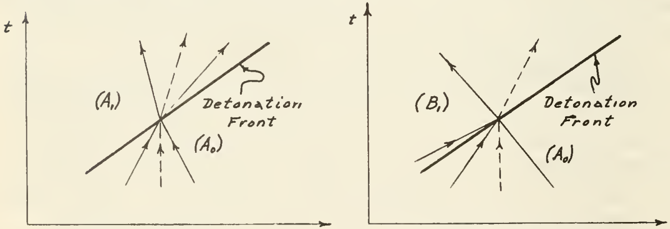
[1] It should be emphasized that the theory as considered in this report, based on the assumption that the reaction front be a sharp discontinuity, does not offer any possibility of predicting whether a detonation or a deflagration will occur in a given situation (except that under certain circumstances deflagration flow is not possible).

[2] The limiting case is the one in which the flame together with the pre-compression shock are just equivalent to a detonation.

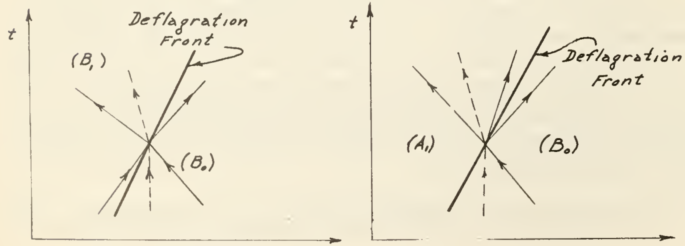
Strong detonations $t = 0$,
Weak detonations $t = 1$,
Weak deflagrations $t = 1$,
Strong deflagrations $t = 2$.

Chapman-Jouguet detonations and deflagrations are here classed with strong detonations or weak deflagrations respectively.

These peculiar under-determinacies are a consequence of Jouguet's important rule (cf.[3]); concerning the properties of the gas flow observed from the reaction front:



Weak detonation. Strong detonation.



Weak deflagration. Strong deflagration.

Particle paths ⇢ and sound paths ↗ at detonation or deflagration fronts.

Figure 1

The flow ahead of a detonation front is supersonic, and subsonic ahead of a deflagration front. The flow is subsonic behind a strong detonation and a weak deflagration front, supersonic behind a weak detonation and a strong deflagration front. The flow is here always understood relative to the reaction front.

We now proceed to discuss the chief aim of the present paper, namely to decide which of the flow processes, still permitted by the conservation laws, are excluded through the action of viscosity, heat conduction, and chemical reaction. To this end we shall take into account that the reaction zone has a finite extension. We then shall set up the differential equations governing the transition across such a reaction zone and investigate under which circumstances these differential equations possess solutions satisfying the boundary conditions imposed at the two ends of the reaction zone. These boundary conditions consist in prescribing the chemical composition, pressure, temperature, and velocity of the gases at both ends of the reaction zone in such a way that the laws of conservation of mass, momentum, and energy are satisfied by these quantities. The differential equations in the interior of the reaction zone express the same conservation laws, but take into account chemical reaction, viscosity, and heat conduction.

Investigations of this kind for shocks not involving a chemical reaction have been made in detail by various authors1). The result was that a transition between the given quantities at both sides of the zone is always possible provided that the direction of the flow corresponds to increasing entropy. Our investigation will show that the same is true for strong detonations and for Chapman-Jouguet detonations. For other modes of reaction, however, the situation is completely different. Here are the results of our analysis:

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1) See e. g. Becker [4] and Weyl [5] .

Unless the rate of reaction is excessively high, weak detonations, though compatible with the conservation laws, are impossible. The condition that the detonation be strong or of the Chapman-Jouguet type is, therefore, the desired additional condition mentioned in the beginning. Consequently, a flow involving a detonation is uniquely determined. For, if the piston velocity is high, $u_p > u_D$, there is a unique solution involving a strong detonation, as mentioned before; for lesser piston velocity, however, $u_p \leq u_D$, there is now only one possible flow left in which the velocity of the burned gas equals the piston velocity, and that is the flow involving a Chapman-Jouguet detonation. In particular we see that for a tube with a closed end, $u_p = 0$, or open end, $u_p << 0$, a Chapman-Jouguet detonation is the only possible one. Thus the occurrence of this particular detonation is here deduced and no additional hypothesis is required.

If, however, the reaction rate is excessively high, the analysis yields the result that the Chapman-Jouguet detonation is impossible. Instead, a particular weak detonation is possible which travels with a well-determined velocity (depending on pressure and temperature in the unburnt gas, reaction rate, viscosity, and heat conductivity). If the piston velocity is large enough, adjustment still requires a strong detonation. For lesser piston velocities, for example for closed or open ends, adjustment is effected by the particular weak detonation followed by an appropriate shock or an appropriate rarefaction wave.

As to deflagrations the results of the analysis are that strong deflagrations are impossible altogether.(1) A weak deflagration is possible only with a well-determined speed. We distinguish the "flame velocity," i.e. the velocity of the reaction front relative to the tube, from the "burning speed," i.e. the speed of

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1) This result could also be established by v. Neumann's argument ignoring viscosity and heat conduction and taking only the finite rate of chemical reaction into account.

the reaction front relative to the unburnt gas ahead of it. While the flame velocity depends on the boundary conditions of the problem as a whole, the burning speed depends only on pressure and temperature in the unburnt gas, and also on reaction rate, heat conductivity and viscosity. That the burning speed has this particular value is the desired additional condition for deflagrations. As stated before, for a burning speed arbitrary within certain limits, a deflagration flow can be found which is adapted to the piston motion. A further limitation is imposed by excluding strong deflagrations. Thus we see: Within certain limits for the data of the problem there exists a uniquely determined flow involving a deflagration and adapted to the piston motion.

We call attention to a number of detailed investigations of the transition process in reaction zones. Detonation transitions have been determined in detail by Eyring and his collaborators1). Deflagration flame speeds have been calculated by Jouguet and others2), on the basis of various assumptions about the details of the transition process. The aim of the present report is different: it is not intended to give new methods for calculating such transition processes. The intention is solely to decide the question of determinacy by investigating such transition processes systematically on the basis of the existing theory.

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1) See [6] for an excessively high reaction rate, [7] for actual reaction rates. the latter paper contains a great number of detailed investigations concerning detonations primarily of solid explosives.

2) Cf. Lewis and v. Elbe [8], Jost [9], Semenov [10], further [11] and [12]; the latter report gives a survey of earlier work.

1. The internal mechanism of the reaction process.

We assume the process to be strictly one-dimensional[1] and observe the process from a frame moving with instantaneous flame or detonation speed. We assume that the flow so observed is steady at the time considered in the neighborhood of the reaction zone[2]. This is in agreement with our basic assumption (p. 3) that the reaction zone is very narrow and of nearly constant width. Consequently, all quantities depend only on an abscissa x, and not on the time. At each place x, there is a mixture of burnt and unburnt gas; we denote by ε the fraction of mass of burnt gas in the mixture. We denote pressure and specific volume by p and τ and introduce the "reduced temperature" $\Theta = p\tau$, a quantity which has the dimension of velocity squared. We assume burnt and unburnt gas to be ideal. Accordingly, Θ is proportional to the temperature[3]. The internal energy e per unit mass of the burnt and of the unburnt gas is assumed to be a function of Θ only, (actually e depends also somewhat on the pressure p, see also footnote[3]; denoting by g the energy of formation per unit mass (at absolute zero temperature), we introduce the total energy per unit mass

$$E = e + g .$$

Burnt and unburnt gas are distinguished by the superscripts (1) and (0). The total energy per unit mass of the mixture is then

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[1] This assumption is no serious restriction for the discussion of the internal mechanism since the flow in the neighborhood of a point of a reaction front may be considered one-dimensional to the same degree of accuracy as the assumption is valid that the reaction front is a sharp discontinuity.

The assumption of the one-dimensional character of the flow is, however, a serious restriction for the external flow problem since this assumption is known to be never quite satisfied for combustion waves.

[2] The assumption of "local steadiness" does by no means imply that we consider only reaction processes that proceed with constant velocity into the unburnt gas. See the discussion in the Appendix.

[3] The absolute temperature is given by $R\Theta/M$ where R is the gas constant and M the molecular weight. We disregard the dependence of the molecular weight on the mixture ratio ε.

$$E^{(\varepsilon)}(\theta) = (1-\varepsilon)E^{(0)}(\theta) + \varepsilon E^{(1)}(\theta) \quad .$$

On the energy functions $E(\theta)$ we require that

$$\frac{\partial E^{(\varepsilon)}}{\partial \varepsilon} < 0$$

or

$$E^{(0)}(\theta) > E^{(1)}(\theta) .$$

This condition implies that the "liberated energy"

$$E^{(0)}(0) - E^{(1)}(0)$$

is positive. (It is convenient to make this assumption although most of our conclusions hold without it.) Our requirement is satisfied if burnt and unburnt gas are "polytropic"; i. e. if the energies are given by

$$E^{(0)}(\theta) = \frac{\theta}{\gamma_0 - 1} + g_0, \; E^{(1)}(\theta) = \frac{\theta}{\gamma_1 - 1} + g_1$$

with constant γ_0, γ_1, g_0, g_1, provided that the temperature is below a certain limit[1] .

By v we denote the velocity of the steady gas flow and by $m = \tau^{-1}v$ the "mass flux" of mixture through a unit cross-section per unit time. By S we denote the mass of burnt gas created per unit mass of unburnt gas per unit time. We assume that the "reaction rate," S, depends on θ and p, (cf. footnote 1) on p.11), and that S vanishes below a certain "safety temperature":

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[1] This limit corresponds to $\theta \leq \frac{(\gamma_0 - 1)(\gamma_1 - 1)}{\gamma_0 - \gamma_1}(g_0 - g_1)$. If one assumes $\gamma_0 = 1.4$, $\gamma_1 \sim 1.2$, the molecular weight $M_0 = M_1 \sim 30$, and the "liberated energy" $g_0 - g_1 \sim .7$ kcal/gr , then the limit is about 3200°K. This case is, however, unrealistic since for such temperatures the value of γ for combustible gases will hardly ever be as high as 1.4.

$$S = 0 \quad \text{for} \quad \theta \leq \theta_S.^{1)}$$

The transition between the two states on both sides of the reaction front is effected by the action of viscosity and heat conduction²⁾. We introduce corresponding coefficients μ and λ such that

$$-\mu \frac{dy}{dx} \quad \text{and} \quad -\lambda \frac{d\theta}{dx}$$

are the viscous pressure and heat per unit mass conducted through a unit cross-section per unit time³⁾. These coefficients depend on p, τ, and ε; but we need pay only little attention to this dependence for our general discussion.

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1) The latter assumption is made only to achieve mathematical simplicity. In recent papers [7], [11], [12], the reaction rate is assumed to be of the form

$$S = S_\infty e^{-A/\theta}$$

where A, proportional to the activation energy, is so large that S is negligible when θ assumes values corresponding to a temperature of 300°K. The reduced safety temperature θ_s has no precise significance (as the ignition temperature had in the older literature); it is simply a value below which S can be set equal to zero for all practical purposes.) The maximal reaction rate, S_∞, may depend on P.

2) We ignore diffusion and radiation. Diffusion should not be neglected in the actual calculation of flame speeds according to [12]. We felt that for the sake of simplicity we could disregard diffusion since the additional terms due to it would not seem to entail any essential change in the general results.

One might object to using the notions viscosity, heat conduction, and diffusion if the width of the transition zone is extremely small. It seems likely, though, that nevertheless our results remain correct in qualitative respects, in particular as far as determinacy is concerned.

3) The customary coefficients of viscosity and heat conduction are, in our notation, $3/4\,\mu$ and λ/R, R being the gas constant such that $R\theta$ is the temperature.

We now formulate the laws governing the process. The continuity equation simply assumes the form

$$(0) \qquad m = \text{const.}$$

The law of conservation of momentum is

$$(1)' \qquad -\mu\frac{dv}{dx} + p + m\,v = P = \text{const.}$$

Conservation of energy1) is expressed by

$$(2)' \qquad -\lambda\frac{d\theta}{dx} + m\left[E^{(\varepsilon)}(\theta) + \frac{1}{2}v^2\right] + v\left[p - \mu\frac{dv}{dx}\right] = m\,Q = \text{const.}$$

The balance between burnt and unburnt gas is given by

$$(3)' \qquad -v\frac{d\varepsilon}{dx} + (1-\varepsilon)\,S(\theta) = 0\,,$$

assuming a first order reaction from a unimolecular mechanism2) .

The problem is to investigate possible solutions of these differential equations if the values of the quantities v, p, τ, and ε are given at the end points of the reaction zone. We modify this problem by prescribing the same values of these quantities at $x = \infty$ and $x = -\infty$. That it is justified with good approximation to substitute the modified problem for the original one follows from our basic assumption (p. 3) that the width of

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1) If we were to consider diffusion we would introduce a coefficient δ such that $-\delta\, d\varepsilon/dx$ is the fraction of mass of burnt gas diffusing through a cross-section per unit time. Then we would have to add the term $\tau d(\delta d\varepsilon/dx)dx$ to equation (3)' and $-\delta d[E^{(\varepsilon)}(\theta)+\frac{1}{2}v^2]/dx$ to equation (2)' in order to express the diffusion of energy. The resulting modified equation (2)' would differ somewhat from those in the literature (see [12] where only the diffusion of the energy of formation is taken into account.

2) If a different mechanism of reaction were assumed leading to terms $(1-\varepsilon)^2 S$ or $(1-\varepsilon)(1+n\varepsilon)S$, cf. [11] and [12], no change in the general conclusions would result.

the reaction zone is very narrow. More specifically, the assumption was that the rate of change of the pertinent quantities outside the reaction zone is negligibly small as compared to the rates of change of these quantities inside the reaction zone. Consequently, these quantities appear to be nearly constant at the ends of the reaction zone over a region whose extension is large compared with the width of the reaction zone. It is then natural to assume that the process inside the reaction zone can very well be approximated by a process that extends over the whole field from $x = -\infty$ to $x = +\infty$ and in which the pertinent quantities assume at $\pm\infty$ those values that are prescribed for the proper process at the ends of the finite reaction zone.[1)]

Accordingly we ask for solutions of the equations $(1)'$, $(2)'$, and $(3)'$ which are defined for $-\infty < x < \infty$ and which approach finite limit values (with $\tau \neq 0$) as $x \rightarrow \pm\infty$; then the derivatives approach zero as seen from $(1)'$, $(2)'$, and $(3)'$. Solutions which behave in that way at $x = \infty$ or $x = -\infty$ will be called "regular" there. The limit values for $x \rightarrow -\infty$ are denoted by p_o, τ_o, θ_o, and ε_o; those for $x \rightarrow \infty$ by p_1, τ_1, θ_1, and ε_1. The boundary conditions then consist in prescribing these values; in particular we prescribe

$$\varepsilon_o = 0, \quad \varepsilon_1 = 1 ,$$

expressing that the gas consists of unburnt gas at $x = -\infty$ and of completely burnt gas at $x = +\infty$. From relation $(3)'$ we then

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1) This procedure, typical for the treatment of "boundary layer phenomena" is always employed for differential equations in which the terms of highest order are multiplied by small factors. (In our case these factors are μ, λ, and S_∞^{-1}).

No accuracy would be gained by trying to discuss the solutions for a finite range $x_o \leq x \leq x_1$; for, the conservation laws $(1)'_\infty$ and $(2)'_\infty$ would not be accurately valid unless accidentally

$$\frac{dt}{dx} = \frac{d\theta}{dx} = \frac{d\varepsilon}{dx} = 0 \text{ at } x = x_o \text{ and } x = x_1 \quad .$$

For the infinite range it follows from regularity (see Section 2) that these derivatives vanish at the end points.

deduce that the flux m is positive:

$$m = m\int_{-\infty}^{\infty} d\varepsilon = \int_{-\infty}^{\infty} (\tau - 1)(1 - \varepsilon)\, \mathcal{S}(\theta) dx > 0 \ .$$

From this fact it follows that the reaction begins in the unburnt gas at $x = -\infty$ and ends in the burnt gas at $x = \infty$.

The values p_o, τ_o, θ_o, v_o, and p_1, τ_1, θ_1, v_1 for unburnt and burnt gas are those that are prescribed at both sides of the discontinuity front. These quantities are not prescribed arbitrarily, they are to satisfy the conservation laws: (0) and

$(1)'_\infty$
$$p_o + m v_o = p_1 + m v_1 = P$$

$(2)'_\infty$
$$E_o + \theta_o + \tfrac{1}{2} v_o^2 = E_1 + \theta_1 + \tfrac{1}{2} v_1^2 = Q \ ,$$

through which at the same time the values of the constants P and Q are determined. Here we have set

$$E^{(o)}(\theta_o) = E_o \text{ and } E^{(1)}(\theta_1) = E_1 \ .$$

The conservation laws follow immediately for any regular solution from the differential equations (1)'and (2)', since these equations reduce to $(1)'_\infty$ and $(2)'_\infty$ for $x = \infty$ and $x = -\infty$.

A further assumption which we impose on our boundary values is

$$\theta_o < \theta_s < \theta_1 \ ,$$

expressing that no reaction can take place in the unburnt gas at its initial temperature, and that reaction would take place at the final temperature if unburnt gas were still left.1)

For the following arguments it is convenient to eliminate v and p by

$$v = m\tau \quad \text{and} \quad p = \tau^{-1}\theta \ ,$$

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1) Relation $\theta_o > \theta_s$ would imply $S > 0$ for $\theta = \theta_o$ and would hence not be compatible with equation (3)' for a regular solution.

and to consider τ, θ and ε as the only dependent variables; the equations then become

$$- \mu m \frac{d\tau}{dx} + \tau^{-1}\theta + m^2\tau = P \quad , \tag{1}$$

$$-\lambda\frac{d\theta}{dx} + m\left[E^{(\varepsilon)}(\theta) - \frac{1}{2}m^2\tau^2 + P\tau\right] = m\,Q \quad , \tag{2}$$

$$- m\frac{d\varepsilon}{dx} + \tau^{-1}(1-\varepsilon)\;S(\theta) = 0 \quad .$$

The constant coefficients m, P, Q, and the boundary values τ_o, τ_1, θ_o, θ_1, $\varepsilon_o = 0$, and $\varepsilon_1 = 1$ are subject to the conservation laws

$$\tau_o^{-1}\theta_o + m^2\tau_o = \tau_1^{-1}\theta_1 + m^2\tau_1 = P \quad , \tag*{$(1)_o$}$$

$$E_o + \theta_o + \frac{1}{2}m^2\tau_o^2 = E_1 + \theta_1 + \frac{1}{2}m^2\tau_1^2 = Q \quad . \tag*{$(2)_o$}$$

We now consider the system of differential equations (1), (2), (3) and ask whether or not it possesses regular solutions assuming the prescribed boundary values.

2. Regularity and determinacy.

We shall introduce as "degree of regularity" for each endpoint a number r such that the manifold of solutions of the differential equations (1), (2), (3) which are regular at that endpoint and assume the prescribed boundary values there depends on r parameters.

Let us first consider the endpoint $x = \infty$. To determine the degree of regularity r_1 at the end $x = \infty$ we shall introduce characteristic exponents, α, by the following formal procedure. We expand the differential equations (1), (2), (3) with respect to powers of $\tau-\tau_1$, $\theta-\theta_1$, and $\varepsilon-\varepsilon_1=\varepsilon-1$. The terms of order zero vanish by definition of P and Q. The terms of first order constitute a system of linear differential equations with constant coefficients, the "linearized" differential equations for $x=\infty$. Upon inserting into these equations multiples of an exponential function $e^{\alpha x}$ for $\tau-\tau_1$, $\theta-\theta_1$, and $\varepsilon-1$, we obtain three linear equations for the three coefficients whose determinant is a cubic equation for α. The three roots of this cubic equation are the three characteristic exponents. We anticipate the fact, shown later on, that for our equations these characteristic exponents are always real. Suppose we have r_1 negative and $3-r_1$ positive characteristic exponents, then r_1 is the degree of regularity. This fact is implied by the well-known theory of singular points of ordinary differential equations. The behavior of the r_1-parametric set of regular solutions can be characterized by the regular solutions of the linearized equations; the latter are a linear combination of exponential functions $e^{\alpha x}$ if the characteristic roots are different; otherwise terms like $xe^{\alpha x}$ or $x^2e^{\alpha x}$ enter. In case one characteristic exponent is zero, one cannot say offhand what the degree of regularity is; a special consideration is needed.

The linearized equations at $x=\infty$ for the quantities $\tau-\tau_1$, $\theta-\theta_1$, $\varepsilon-1$ are immediately found to be

$$(1)^+ \qquad m\mu_1\frac{d(\tau-\tau_1)}{dx}+\tau_1^{-2}\theta_1(\tau-\tau_1)-m^2(\tau-\tau_1)-\tau_1^{-1}(\theta-\theta_1)=0,$$

$$(2)^+ \qquad \lambda_1\frac{d(\theta-\theta_1)}{dx}-m\left\{\frac{\theta-\theta_1}{\gamma_1-1}-\Delta E_1(\varepsilon-1)+\tau_1^{-1}\theta_1(\tau-\tau_1)\right\}=0,$$

$$(3)^+ \qquad m\frac{d(\varepsilon-1)}{dx}+\tau_1^{-1}S_1(\varepsilon-1)=0,$$

where we have set $\frac{1}{\gamma-1}=\frac{\partial E^{(\varepsilon)}(\theta)}{\partial\theta}$, $\Delta E=E^{(0)}-E^{(1)}$, and the subscript (1) indicates that these quantities and also μ, λ, and S, are to be taken for $\theta = \theta_1$, $\tau = \tau_1$, $\varepsilon = 1$.

For the characteristic exponent α one then obtains the equation

$$\begin{vmatrix} m\mu_1\alpha - m^2 + \tau_1^{-2}\theta_1 & -\tau_1^{-1} & 0 \\ -m\tau_1^{-1}\theta_1 & \lambda_1\alpha - \frac{m}{\gamma_1 - 1} & m\Delta E_1 \\ 0 & 0 & m\alpha + \tau_1^{-1}S_1 \end{vmatrix} = 0$$

or

$$[m\tau_1\alpha + S_1][m\tau_1^2\lambda_1\mu_1\alpha^2 - (m^2\tau_1^2\lambda_1 - \theta_1\lambda_1 + m^2\tau_1^2\frac{\mu_1}{\gamma_1 - 1})\alpha - \frac{m}{\gamma_1 - 1}(\gamma_1\theta_1 - m^2\tau_1^2)] = 0 \tag{4}$$

The first bracket has evidently one negative root. As to the second bracket, which we write in the form $a\alpha^2 - b\alpha + c$ we observe that it has real roots since the discriminant

$$b^2 - 4ac = (m^2\tau_1^2\lambda_1 - \theta_1\lambda_1 + m^2\tau_1^2\frac{\mu_1}{\gamma_1 - 1})^2 + 4\,\frac{m^2\tau_1^2\lambda_1\mu_1}{\gamma_1 - 1}(\gamma_1\theta_1 - m^2\tau_1^2)$$

$$= (m^2\tau_1^2\lambda_1 - \theta_1\lambda_1 - m^2\tau_1^2\frac{\mu_1}{\gamma_1 - 1})^2 + 4m^2\tau_1^2\lambda_1\mu_1\theta_1$$

is positive.

Since $a > 0$ we see that the second bracket has one positive and one negative root if $c < 0$. If $c = 0$, we have $b = b_o = (\gamma_1 - 1)\theta_1\lambda_1 + \frac{\gamma_1}{\gamma_1 - 1}\theta_1\mu_1 > 0$ and hence the bracket has one vanishing and one positive root. If $c > 0$ we have $b > b_o > 0$ and hence the bracket has two positive roots.

In case $c < 0$ we have $r_1 = 2$ and in case $c > 0$ we have $r_1 = 1$. A detailed investigation of the vector field corresponding to the differential equation would show that in case $c = 0$ a two parametric set of regular solutions exists; hence $r_2 = 2$ also in this case. Since the condition $c \gtrless 0$ is equivalent with $\gamma_1 \theta_1 \gtrless m^2 \tau_1^2$ we have to distinguish the following two cases

$$\text{Case } (A_1) \qquad m^2\tau_1^2 > \gamma_1\theta_1 \ ,$$

$$\text{Case } (B_1) \qquad m^2\tau_1^2 \leqq \gamma_1\theta_1 \ .$$

The degree of regularity in these cases is:

$$\text{Case } (A_1) \qquad r_1 = 1 \ ,$$

$$\text{Case } (B_1) \qquad r_1 = 2 \ .$$

Employing the sound speed $c_1 = \sqrt{\gamma_1 \theta_1}$ for the burnt gas in state (1) we can write the condition for cases (A_1) and (B_1) in the form

$$\text{Case } (A_1) \qquad v_1 > c_1 \ ,$$

$$\text{Case } (B_1) \qquad v_1 \leqq c_1 \ .$$

Thus the flow of the burnt gas in state (1) is supersonic in case (A_1) and subsonic or sonic in case (B_1).

For the state (o) at the end $x = -\infty$ we obtain a similar equation for α, the only difference being that $S = 0$ in state (o) since $\theta_o \leqq \theta_S$ was assumed. The equation for α then becomes

$$(4)^- \qquad m\alpha\Big[m\tau_o^2\lambda_o\mu_o\alpha^2 - (m^2\tau_o^2\lambda_o - \theta_o\lambda_o + m^2\tau_o^2\frac{\mu_o}{\gamma_o - 1})\alpha$$

$$- \frac{m}{\gamma_o - 1}(\gamma_o\theta_o - m^2\tau_o^2)\Big] = 0 \ ,$$

where λ_0, μ_0, γ_0 refer to $\theta = \theta_0$, $\tau = \tau_0$, $\varepsilon = 0$. The first factor here has the root $\alpha = 0$. The bracket always has one positive root and in addition one positive, vanishing, or negative root depending on whether $\gamma_0\theta_0 - m^2 \, {}^2_0 > 0, = 0,$ or < 0.

To determine the degree of regularity r_0 at the end $x = -\infty$ we first recall that $\theta_0 < \theta_s$ was assumed. Hence for every regular solution assuming the prescribed boundary values at $x = -\infty$, we have $\theta < \theta_s$ if x is sufficiently negative, for $-\infty < x \leq x_s$ say. By virtue of $S = 0$ for $\theta \leq \theta_s$ equation (3) entails $\varepsilon = 0$ for $-\infty < x \leq x_s$. The investigation of the manifold of solutions regular at $x = -\infty$ is thus reduced to the investigation of the regular solutions of equation (1) and (2) with $E^{(\varepsilon)}(\theta) = E^{(0)}(\theta)$. The characteristic exponents for this problem are the roots of the bracket in relation $(4)^-$. Hence we conclude: If both roots of the bracket are positive we have $r_0 = 2$. The same is true if one of the roots is zero, as a detailed investigation of the vector field corresponding to the differential equation would show. If one of the roots is negative, however, the other one being positive, we have $r_1 = 1$. Accordingly, we distinguish the following two cases:

$$\text{Case } (A_0) \quad m^2\tau_0^2 \geq \gamma_0\theta_0 \; ,$$

$$\text{Case } (B_0) \quad m^2\tau_0^2 < \gamma_0\theta_0 \; .$$

The degree of regularity is

$$r_0 = 2 \quad \text{in case } (A_0) \; ,$$

$$r_0 = 1 \quad \text{in case } (B_0) \; .$$

Employing the sound speed c_0 in the unburnt gas we write the condition for cases (A_0) and (B_0) in the form

$$\text{Case } (A_0) \quad v_0 \geq c_0 \; ,$$

$$\text{Case } (B_0) \quad v_0 < c_0 \; .$$

Thus, the flow of the unburnt gas at $x = -\infty$ is supersonic or sonic there in case A_0, while it is subsonic in case B_0.

We see that four different cases are to be distinguished according to whether case A or case B obtains at $x = \infty$ or at $x = -\infty$. It is now very interesting that by virtue of Jouguet's rule (see Supplement [3], p. 10) these four cases just correspond to the four cases of strong and weak detonations and deflagrations; the Chapman-Jouguet detonation or deflagration, characterized by $v_1 = c_1$, is here classed with the strong detonations or weak deflagrations respectively.

We now shall determine in a formal way, simply by counting the number of parameters, the manifold of solutions which are regular at both endpoints. The set of solutions which are regular at $x = \infty$ is r_1-parametric. Among these solutions those are to be selected which are regular at $x = -\infty$. Since all solutions regular at $x = -\infty$ form a r_0- parametric set in the three-parametric set of all solutions, it is clear that the condition to be regular at $x = -\infty$ is expressed by $3-r_0$ relations. Thus $3-r_0$ conditions are imposed on the r_1 parameters characterizing the solutions regular at $x = \infty$. One of these parameters can always be chosen arbitrarily (within limits), since from every solution satisfying the boundary conditions one obtains a set of others by substituting $x + \text{const.}$ for x. Thus $3-r_0$ conditions are imposed on r_1-1 parameters. If $r_1 - 1 > 3-r_0$, an $(r_0 + r_1 - 4)$-parametric set of solutions can be expected to exist. If $r_1 - 1 = 3-r_0$, one solution (or else a finite number of them) can be expected to exist. If $r_1 - 1 < 3 - r_0$ more conditions are imposed than parameters are available. These conditions will be satisfied only if the coefficients entering the differential equations or the boundary values assume appropriate values. In other words, $4 - r_0 - r_1$ conditions are imposed on coefficients and boundary values. We term the number

$$s = 4-r_0 - r_1$$

the "degree of over-determinacy." From Jouguet's rule and the determination of the values of r_0 and r_1 given before we find

Strong detonation,	case (A_0B_1),	$s = 0$
Weak detonation ,	case (A_0A_1),	$s = 1$
Weak deflagration,	case (B_0B_1),	$s = 1$
Strong deflagration,	case (B_0A_1),	$s = 2$.

Upon comparing this table with the table for the degree of under-determinacy given in the introduction (p. 6) we realize the fundamental fact that *the degree of over-determinacy resulting from the internal mechanism of the reaction process equals the degree of under-determinacy of the external problem flow*. The number of conditions needed to make the flow problem unique thus equals the number of conditions imposed by the mechanism of the reaction process.

This result may be interpreted as follows: All strong detonations are possible. Weak or Chapman-Jouguet detonations are only possible if one of the parameters of the process satisfies one condition. As such parameter we may consider the flux m. As we shall see later, weak detonations exist just for such values of the flux that lead to Chapman-Jouguet detonations except for sufficiently high values of the reaction rate, for which a larger value of the flux leads to a possible weak detonation. Weak deflagrations are also only possible if one of the parameters, the flux m say, satisfies one condition. As we shall see later, weak deflagrations exist indeed for only a particular value of the flux. Strong deflagrations should exist only if two conditions are satisfied by the parameters. As we shall see later, strong deflagrations do not exist at all.

It must be emphasized that these statements are so far derived in a purely formal manner. They are obtained by balancing the number of available parameters with the number of conditions imposed. A definite statement about existence and uniqueness cannot be made on this basis. As a matter of fact these arguments are not sufficient to exclude weak detonations and strong deflagrations. More detailed considerations are needed for this purpose. In the following Sections (3 and 4) we shall first investigate certain limiting cases of weak deflagrations and strong detonations, and then proceed to discuss in Section 5 the problem of existence of solutions in general.

3. Weak deflagrations.

The degree of over-determinacy was found to be $s = 1$ for weak deflagrations. As indicated above, such deflagrations can therefore be expected to exist only if the coefficients of the differential equations satisfy one condition. This condition may be considered a condition for the constant m, the flux, or for the burning velocity $v_o = \tau_o m$. The question arises whether or not to given values of τ_o, θ_o, and given functions $S(\theta)$ and $E^{(\varepsilon)}(\theta)$ there really is a value of the flux m for which the problem has a solution. We shall deal with this question in Section 5.

Here we shall consider only the limiting case of a constant pressure deflagration in which this question can easily be answered. This limit case results if either heat conductivity λ and viscosity μ approach zero, if the reaction rate S approaches zero[1], or if the pressure p_o increases indefinitely while the temperature θ_o remains fixed. This limit case, to which actual situations frequently come very near, has always been assumed for numerical determinations of the flame speed (see [11],[12]).

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[1] For example by letting $S_\infty \rightarrow 0$, (cf. footnote on p. 12).

The objection may be raised that for small values of the reaction rate the basic assumption (pp. 3 and 10) cannot be satisfied. Nevertheless it is necessary to consider the limit $S \rightarrow 0$ for the discussion of the mathematical implications of the problem formulated in Section 1.

To describe the limiting "constant pressure problem" we first introduce dimensionless quantities

$$\tilde{m} = m\tau_o/\sqrt{\theta_o}$$

$$\tilde{\mu} = \mu S_\infty/p_o\tilde{m}^2 \quad , \quad \tilde{\lambda} = S_\infty/p_o\tilde{m}^2 \ ,$$

$$\tilde{P} = P/p_o \quad , \tilde{Q} = Q/\theta_o \quad ,$$

and introduce the new variables

$$\tilde{x} = x\,S_\infty/m\tau_o \quad ,$$

$$\tilde{\tau} = \tau/\tau_o \quad , \quad \tilde{\theta} = \theta/\theta_o \quad .$$

The equations (1), (2), (3) then become

$$\begin{aligned} -\tilde{\mu}\tilde{m}^2 d\tilde{\tau}/d\tilde{x} + \tilde{\theta}/\tilde{\tau} + \tilde{m}^2\tilde{\tau} &= \tilde{P} \\ -\tilde{\lambda}\, d\tilde{\theta}/d\tilde{x} + E^{(\varepsilon)}(\theta_o\tilde{\theta})/\theta_o - \tfrac{1}{2}\tilde{m}^2\tilde{\tau}^2 + \tilde{P}\tilde{\tau} &= \tilde{Q} \\ -\, d\varepsilon/d\tilde{x} + \tilde{\tau} - 1(1-\varepsilon)\, S(\theta_o\tilde{\theta})/\theta_o &= 0 \quad . \end{aligned}$$

This system of differential equations depends on the parameters $\tilde{m}$, $\tilde{\lambda}$, $\tilde{\mu}$, $\tilde{P}$, $\tilde{Q}$, and θ_o. We obtain the limiting problem by considering a set of such systems for which $\tilde{m}$ approaches zero while the other parameters are kept fixed. In other words: The differential equations of the limiting problem are simply obtained by omitting the three terms involving the factor $\tilde{m}^2$.

The fact that $\tilde{\lambda}$ and $\tilde{\mu}$ are fixed while $\tilde{m}$ approaches zero evidently implies $\lambda S_\infty/p_o \to 0$ and $\mu S_\infty/p_o \to 0$. The limiting equations will therefore represent a good approximation if $\lambda S_\infty/p_o$, $\mu S_\infty/p_o$, and $\tilde{m}$ are small. In that case we can reintroduce the original quantities. Thus we obtain the equations of the constant pressure problem in the following form:

$$(\tilde{1}) \qquad p = P = p_o$$

$$(\tilde{2}) \qquad -\lambda\frac{d\theta}{dx} + m\,[E^{(\mathcal{E})}(\theta) + \theta] = m\,Q \quad ,$$

$$(\tilde{3}) \qquad -m\,\frac{d}{dx} + p\theta^{-1}\,(1 - \mathcal{E})S(\theta) = 0 \quad .$$

where we have eliminated τ from (2) and (3), using $(\tilde{1})$.

Relation $(\tilde{1})$ expresses the fact that under the conditions of the limiting problem the pressure does not vary across the flame front: we have constant pressure combustion. Further we see that the term representing the kinetic energy has dropped out from (2).

The boundary conditions are $\theta = \theta_1$, $\mathcal{E} = 1$ at $x = \infty$, and $\mathcal{E} = 0$ at $x = -\infty$. The constant Q is given by $Q = E_1 + \theta_1$. The relation $E_o + \theta_o = Q$, which holds for regular solutions determines the value $\theta = \theta_o$ at $x = -\infty$.

To investigate possible solutions of this problem one may consider θ as independent variable running from θ_o to θ_1 and combine the equations to

$$(5) \qquad \frac{d\mathcal{E}}{d\theta} \quad \frac{p\lambda}{m^2}\,\frac{S(\theta)}{\theta}\,\frac{1 - \mathcal{E}}{E_1 + \theta_1 - E^{(\mathcal{E})}(\theta) - \theta}$$

It is immediately seen that this equation has a saddle-singularity at the point $\theta = \theta_1$, $\mathcal{E} = 1$. There is just one solution curve that enters this point from the region $\mathcal{E} < 1$, $\theta < \theta_1$. If this curve is followed backwards it will enter the axis $\mathcal{E} = 0$ at a point with $\theta > \theta_s$ provided $p_o\lambda/m^2$ is sufficiently large; if $p_o\lambda/m^2$ is sufficiently small the curve will enter the line $\theta = \theta_s$ at a point with $\mathcal{E} > 0$. It is thus clear that there is just one value of $p_o\lambda/m^2$ for which the curve enters the line $\theta = \theta_s$ with $\mathcal{E} = 0$. Since $d\mathcal{E}/d\theta = 0$ for $\theta \leq \theta_s$, the curve will enter the line $\theta = \theta_o$ also with the value $\mathcal{E} = 0$. That for this solution the quantity x approaches ∞ as $\theta \rightarrow \theta_1$ and $-\infty$ as $\theta \rightarrow \theta_o$ is immediately seen from $(\tilde{2})$ and $(\tilde{3})$.

Thus it is shown that in the limit, as the quantities $\lambda S_\infty/p_o$ and $\mu S_\infty/p_o$ approach zero, a deflagration process exists with a welldefined flux m and flame speed v_o. As will be shown later (at the end of Section 5), the same is true for small values of these quantities, in other words, for sufficiently small values of $\lambda S_\infty/p_o$ and $\mu S_\infty/p_o$ a deflagration exists which is nearly a constant pressure combustion and which is characterized by a uniquely defined burning speed v_o.

Computations of the burning speed can be carried out by solving equations $(\tilde{2})$ and $(\tilde{3})$ or $(\tilde{5})$ through interactions, (see [10], and [11], in the latter report the term $d(\delta\, d\varepsilon/dx)dx$ was added to equation (3) in order to take diffusion into account); it was found in the quoted reports that for the actual situations considered the approximation involved in (2) and (3) was rather accurate since the omitted terms turned out to be very small for the calculated solution.

It is interesting that essentially only the combination $p\lambda/m^2$ or the dimensionless combination

$$(6) \qquad m^2\theta_o/p\lambda S_\infty = (v_o^2/\theta_o)/(\lambda S_\infty/p)$$

enters the constant pressure problem, as seen from equation (5). (More precisely, the problem depends only on the dimensionless quantity (6) in addition to the functions $S(\theta)/S_\infty$ and $E^{(\varepsilon)}(\theta)/\theta_o$; note $E_o + \theta_o = E_1 + \theta_1$.) The quantity (6) approaches a finite limit value as $\lambda S_\infty/p_o$ approaches zero. Therefore, for small values of $\lambda S_\infty/p_o$, the flux m is proportional to $\sqrt{p_o\lambda S_\infty/\theta_o}$ and the burning speed v_o to $\sqrt{\lambda S_\infty\theta_o/p_o}$. If in particular λ, S_∞, and the reduced initial temperature θ_o are kept fixed, the flux increases like $\sqrt{S_\infty/p_o}$ and the burning speed decreases like $\sqrt{S_\infty/p_o}$ as p_o increases. If S_∞ were independent of p or increased with p_o of less than first order, the latter result would mean that the burning speed sgould decrease with increasing pressure. This does not seem to be confirmed experimentally[1]. It is thus indicated that S_∞ increases with p_o of higher than first order. What happens when p_o decreases cannot be derived by considering expression (6), since the approximation made is no longer valid if $p_o/\lambda S_\infty$ is small. Whether or not deflagrations are then possible will be discussed later on, in Section 5.

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[1] See e.g. [9] p. 146, Table 27.

4. Strong detonations and Chapman-Jouguet detonations.

We next consider strong detonations, including Chapman-Jouguet detonation; according to Jouguet's rule they have it in common with weak deflagrations that the flow of the burnt gas is subsonic. The flow of the unburnt gas, however, is supersonic (or sonic). The degree of over-determinacy was found to be $s = 0$. Hence no conditions need be imposed on the data other than the inequality $m^2\tau_1^2 \leq \gamma_1\theta_1$, or $v_1 \leq c_1$. Whether or not it is true under this condition that a unique solution exists will be discussed in the next Section, 5.

In the present Section we shall consider a limiting case obtained by letting $\mu S_\infty/p_o$ and $\lambda S_\infty/p_o$ approach zero. We imagine, in particular that viscosity μ and heat conductivity λ approach zero while S_∞ and p_o are kept fixed. This limiting problem presents an analogy to the limiting problem considered in Section 3; the limiting behavior of the present limiting problem is, however, quite different from that encountered in Section 3.

Consider a sequence of solutions. There are two possibilities: either the terms $\mu\frac{d\tau}{dx}$ and $\lambda\frac{d\theta}{dx}$ in equations (2) drop out in the limit, or $\frac{d\tau}{dx}$ and $\frac{d\theta}{dx}$ become infinite. For those values of x for which the first case occurs, the equations

$$(1)_\infty \qquad \tau^{-1}\theta + m^2\tau = P \, ,$$

$$(2)_\infty \qquad E^{(\varepsilon)}(\theta) - \frac{1}{2}m^2\tau^2 + P\tau = Q \, ,$$

$$(3) \qquad -m\frac{d\varepsilon}{dx} + \tau^{-1}(1-\varepsilon)\,S(\theta) = 0 \, ,$$

are satisfied in the limit. If the second case occurs at a place x, a discontinuity of τ and θ occurs in the limit while ε remains continuous. Such a discontinuity would simply be a shock not involving a reaction.

A more detailed investigation (see Section 5) of the limit process $\lambda S_\infty/p_0$, $\mu S_\infty/p_0 \to 0$ will yield that a strong detonation can in the limit be described as a shock, not involving a reaction, immediately followed by a reaction process governed by equations $(1)_\infty$, $(2)_\infty$, (3). This confirms the accepted idea about a detonation process, which was formulated more specifically by G. I. Taylor and v. Neumann (see [1], e.g.).

The question arises whether to given values of τ_0, θ_0, τ_1, θ_1, and m with $\tau_0^{-1}c_0 < m \leq \tau_1^{-1}c_1$ satisfying the conservation laws, a transition process exists which consists of a shock followed by a reaction. We assume that the temperature to which the shock raises the unburnt gas is above safety temperature. Otherwise the reaction process would simply be a deflagration process, which cannot exist in the present limiting case[1]. Denoting the quantities past the shock front by an asterisk we require

$$\theta_0 < \theta_s < \theta_* \quad .$$

To find out whether the equations $(1)_\infty$, $(2)_\infty$, (3) possess a solution we determine τ and θ as functions of ε from $(1)_\infty$ and $(2)_\infty$, and insert in (3). This is possible if the Jacobian

$$J = \frac{dE^{(\varepsilon)}}{d\theta}\,(m^2 - \tau^{-2}\theta) - \tau^{-2}\theta$$

of $(1)_\infty$ and $(2)_\infty$ does not vanish. Introducing quantities $\gamma^{(\varepsilon)}$ and $c_{(\varepsilon)}$ by

$$dE^{(\varepsilon)}/d\theta = 1/(\gamma^{(\varepsilon)} - 1) \quad ,$$

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[1] Expressing τ and θ through ε by $(1)_\infty$ and $(2)_\infty$, equation (3) becomes a differential equation for ε, which yields $d\varepsilon/dx = 0$ for $\varepsilon = 0$ since $S(\theta_0) = 0$ for $\theta_0 \leq \theta_s$. The sole solution of this differential equation vanishing for $x = -\infty$ is therefore $\varepsilon = 0$.

$$c_{(\varepsilon)}^2 = \gamma^{(\varepsilon)}\theta \quad ,$$

we find

$$J = (m^2 - \tau^{-2}c^2)/(\gamma - 1) \quad ,$$

where τ, c, and γ depend on ε. Since the flow is subsonic in the state (*) past the shock we have $J_* < 0$. In the neighborhood of the state (*) we may therefore express τ and θ in terms of ε and the solution of the equation resulting from (3) is uniquely determined through the initial condition $\varepsilon = 0$ at $x = 0$, say, where we may place the shock front. The question then is whether on continuing the solution one would obtain a value for which J changes sign. The final state is also subsonic, $J_1 < 0$, and the transitions from the state (*) to any of the intermediate states between (*) and (1) correspond, as regards the conservation laws, to a set of weak deflagrations. All the intermediate states are thus subsonic. Consequently, J remains negative throughout[1].

The differential equation for ε resulting from (3) possesses, therefore, a solution with $\varepsilon = 0$ for $x = 0$. Since for this solution, $d\varepsilon/dx \rightarrow 0$ as $\varepsilon \rightarrow 1$, the final state (1) is approached as $x \rightarrow \infty$. Thus it is seen that a limiting type detonation consisting of a shock followed by a reaction is possible for arbitrary values of the flux m, satisfying $\tau_0^{-1}c_0 < m \leq \tau_1^{-1}c_1$.[2]

The reaction process in a strong (limit type) detonation following the shock has it in common with a weak deflagration that unburnt gas in a subsonic state is transformed into burnt gas in a subsonic state. The two processes differ, however, in other respects. The initial temperature in a deflagration is below safety temperature while the reaction in a detonation begins with a higher temperature. Also in a deflagration the rates of change $d\tau/dx$, $d\theta/dx$, $d\varepsilon/dx$ are zero initially while there is no such restriction for the reaction process following a shock; for small values of λ and μ the rates of change undergo such great changes in the narrow shock zone that adjustment to any values of these rates at the beginning of the reaction zone is possible. It can thus be understood that for the reaction process in a detonation no definite value of the flux is required as for proper deflagrations.

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[1] Whether or not $\partial E^{(\varepsilon)}/\partial\varepsilon$ changes sign during this process is immaterial, cf. however, v. Neumann's report [1], in which transition processes are discussed on the basis of equations $(1)_\infty$ and $(2)_\infty$.

[2] For numerical determination of such processes and various detailed discussions see the reports by Eyring and his collaborators, [6](where an excessively high reaction rate was assumed) and [7]. (The case shown in Fig. 10a, p. 44 in [7] and labeled "steady deflagration" there is a "weak detonation" in our terminology.)

5. Discussions of possible processes with the aid of the vector field.

It is very helpful for the further discussion to refer to the vector field in the $(\tau, \theta, \varepsilon)$-space generated by the differential equations (1), (2), and (3). It is convenient for our discussion to consider as positive the direction of decreasing x; when we speak of following a solution curve $\mathcal{S}$ we always imply that we travel in direction of decreasing x. All vectors of the field point to smaller values of ε except on the surfaces $\varepsilon = 1$ and in the region $\theta \leq \theta_s$, where they lie in the surfaces $\varepsilon = \text{const}$. Every solution curve that hits the surface $\theta = \theta_s$ will stay on the plane $\varepsilon = \text{const.}$ from there on.

Further important properties of this vector field are these: $d\tau = 0$ on the cylinder $\theta + m^2\tau^2 = P\tau$ and $d\theta = 0$ on the surface ξ given by the equation

$$E^{(\varepsilon)}(\theta) = \frac{1}{2}m^2\tau^2 - P\tau + Q_0 .$$

Points of intersections of the surface ξ with the cylinder $\theta + m^2\tau^2 = P\tau$ and the plane $\varepsilon = \text{const.}$ will be denoted by A_ε

and B_ε . The conservation laws $(1)_\infty$ and $(2)_\infty$ are obviously satisfied at such points. Any two such points on the plane ε = const. with $\theta > 0$ and $\tau > 0$ evidently represent the two states on both sides of a possible shock transition in the gas mixture characterized by the value of ε considered. Therefore, one of these two points, A_ε , corresponds to a supersonic, the other, B_ε , to a subsonic flow. We assume the values of the constants P and Q such that the surface ξ intersects the initial plane $\varepsilon = 0$ at two points A_0 and B_0 with $\theta > 0, \tau > 0$. From the discussion on p.28 it follows that for every $\varepsilon > 0$ two points of intersection A_ε and B_ε exist as long as A_ε or B_ε do not become sonic, or, what is equivalent, do not coalesce. We assume that this is not the case for $0 \leq \varepsilon < 1$; this assumption is primarily a condition on the flux m. We also assume that $\theta > 0$, $\tau > 0$ at these points for $0 \leq \varepsilon \leq 1$. We then have two curves $\mathcal{A}$ and $\mathcal{B}$ of points A_ε and B_ε along which θ and τ are continuous functions of the parameter ε. (The last assumption made here is somewhat stronger than necessary. For the discussion of weak deflagrations, for example, only the existence of the curve $\mathcal{B}$ is needed. Incidentally, the existence of the supersonic state A_ε with $\theta > 0, \tau > 0$ always implies the existence of the subsonic state B_ε , but the converse is not true.)

At the points A_ε, B_ε we have $d\tau = d\theta = 0$, $d\varepsilon/dx > 0$ except for $\varepsilon = 1$ or $\theta \leq \theta_s$; hence the field vector points in the negative ε- direction at these points. The projections of the field vectors on the planes ε = const. have singularities at the points A_ε and B_ε . At a point A_ε the projected field has a nodal point and the solution curves of the projected field lead from the neighborhood of this point into it. At the point B_ε the projected field has a saddle-singularity; (see Figures 2 to 5). At the points A_ε and B_ε on the surface $\varepsilon = 1$ and in the region $\theta \leq \theta_s$ the three-dimensional vector field has singularities.

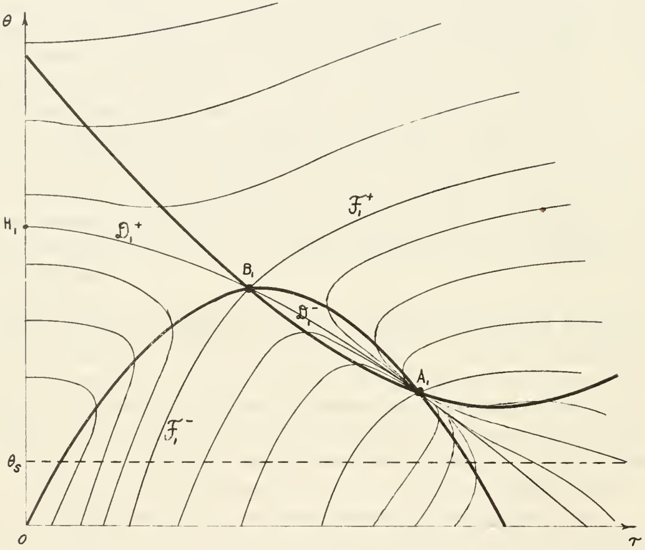

Fig. 2

Detonation

(Integral curves of the projected vector field on the plane $\mathcal{E} = 1$ for a detonation)

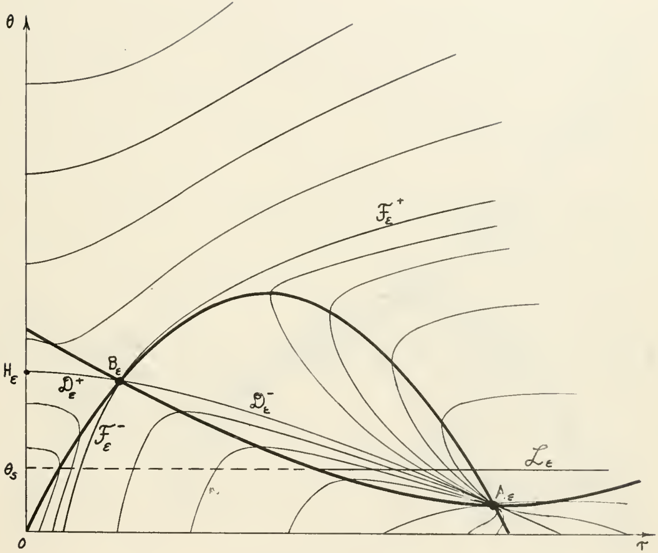
θ
H_ε
θ_s
0
τ
B_ε
A_ε
$\mathcal{D}_\varepsilon^+$
$\mathcal{D}_\varepsilon^-$
$\mathcal{F}_\varepsilon^+$
$\mathcal{F}_\varepsilon^-$
$\mathcal{L}_\varepsilon$

Fig. 3
Detonation
(Integral curves of the projected vector field on the plane $\mathcal{E}$ = const. for a detonation)

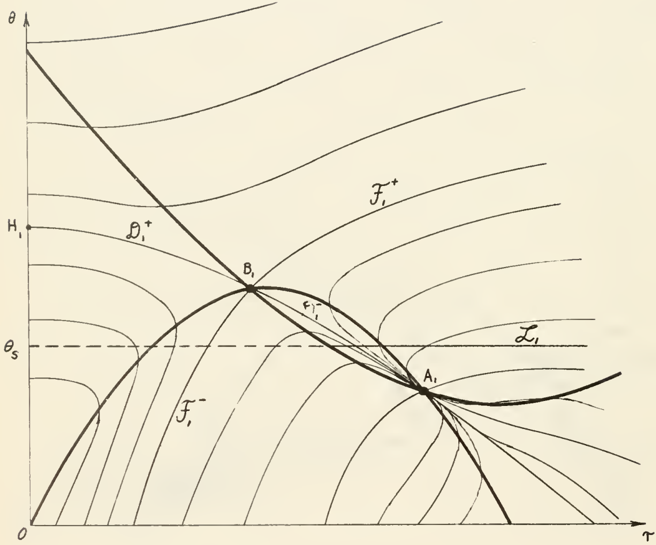

Fig. 4

Deflagration

(Integral curves of the projected vector field on the plane $\mathcal{E} = 1$ for a deflagration)

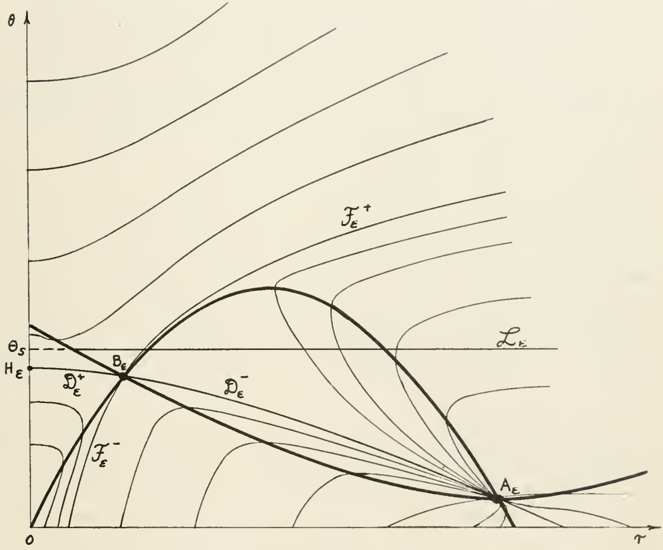
θ
θ_S
H_ε
B_ε
$\mathcal{D}_\varepsilon^+$
$\mathcal{D}_\varepsilon^-$
$\mathcal{F}_\varepsilon^+$
$\mathcal{F}_\varepsilon^-$
$\mathcal{L}_\varepsilon$
A_ε
0
τ

Fig. 5
Deflagration

(Integral curves of the projected vector field on the plane ε = const. for a deflagration)

If we are interested in a deflagration we must assume that $\theta < \theta_s$ for the initial point B_o, (see p.27); if we are interested in a detonation we must assume,(see p.28 and Figs.2,3), that $\theta > \theta_s$ at the point B_o, which in this case is connected with the initial point A_o through a curve representing a shock. We require somewhat more for detonations, viz. that $\theta > \theta_s$ on the whole line $\mathcal{B}$. We first investigate which strong deflagrations and weak detonations are possible. Both processes have it in common that the flow in the burnt gas is supersonic. The state (1) thus belongs to the case (A), and corresponds to a point A_1. As was shown earlier there exists in case (A_1) only a one-parametric set of solutions which are regular at $x = \infty$, and the values of the parameter may be chosen arbitrarily provided it is so chosen that ε decreases as x decreases. Thus there exists only one solution curve, $\mathcal{C}$, starting at A_1 which could represent one of the processes mentioned. If this solution curve $\mathcal{C}$ reaches the point B_o it represents a strong deflagration, if it reaches the point A_o it represents a weak detonation.

In the following we shall consider problems differing in the reaction rate S, all other parameters being unaltered; we may, for example, assume the factor S_∞ (cf.1 on p. 12) to vary from 0 to ∞. The curves $\mathcal{A}$ and $\mathcal{B}$ are evidently independent of S; the curve $\mathcal{C}$, however, depends on S. If we want to emphasize this dependence we write (S).

If the reaction rate S is very high compared with p_o/λ and p_o/μ, all vectors point nearly in negative ε-direction except near $\varepsilon = 1$ and $\theta \leq \theta_s$. In this case, therefore any solution curve is approximately a straight line in the negative ε-direction until it meets the surface $\theta = \theta_s$. Therefore, the curve $\mathcal{C}$ that begins at the point A_1, i. e. at $\varepsilon = 1$, $\theta = \theta_1$, $\tau = \tau_1$, ends up on $\varepsilon = 0$ nearly with the values $\theta = \theta_1$, $\tau = \tau_1$, hence with nearly $\theta = \theta_1 > \theta_s$. Thus we see that $\mathcal{C}$ ends up on $\varepsilon = 0$ at a point with $\theta > \theta_s$ if S is sufficiently high. At such a point $d\varepsilon/dx > 0$ and hence there is no continuation of the curve on the plane $\varepsilon = 0$ and hence none of the desired initial states is reached.

Let us consider the opposite extreme that the reaction rate S is very small; then the direction of the field vector lies everywhere nearly in the plane $\varepsilon =$ const. except near the curves $\mathcal{A}$ and $\mathcal{B}$. Consider any "cylindrical" neighborhood of the line $\mathcal{A}$ and exclude from it an arbitrarily small neighborhood of the point A_1. If S is small enough then clearly the vector field on the lateral surface of the "cylinder" points into its interior. The curve $\mathcal{C}$, beginning at A_1, can therefore never lead far away from the curve $\mathcal{A}$; for, as soon as moved away from $\mathcal{C}$, the rate of change $d\varepsilon/dx$ would become much smaller than $|d\tau/dx| + |d\theta/dx|$ and therefore the curve $\mathcal{C}$ would again be drawn nearer into the neighborhood of $\mathcal{A}$. Consequently, the curve $\mathcal{C}$ meets the surface $\theta = \theta_s$ not far from the intersection A^s of this surface with the curve $\mathcal{A}$, remains from there on the plane $\varepsilon =$ const and soon enters the point A_ε.

In general the course of the curve $\mathcal{C}$ can be delimited as follows: Let $(\tau_\varepsilon, \theta_\varepsilon)$ be the coordinates of the point A_ε. From the assumption $\partial E^{(\varepsilon)}/\partial\varepsilon > 0$ made earlier (p.20) it follows that τ_ε increases and θ_ε decreases with decreasing ε.1) The statement

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1) From (1) and (2) we have

$$\frac{d\theta_\varepsilon}{\gamma_\varepsilon - 1} + \frac{\partial E^{(\varepsilon)}}{\partial\varepsilon}\, d\varepsilon = -\tau_\varepsilon^{-1}\theta_\varepsilon\, d\tau_\varepsilon \quad ,$$

$$d\theta_\varepsilon = -\,(m^2\tau_\varepsilon - \tau_\varepsilon^{-1}\theta_\varepsilon)\,d\tau_\varepsilon$$

where $P = \tau_\varepsilon^{-1}\theta_\varepsilon + m^2\tau_\varepsilon$ has been used. Eliminating $d\theta_\varepsilon$ one has

$$(\gamma_\varepsilon - 1)\frac{\partial E^{(\varepsilon)}}{\partial\varepsilon}\, d\varepsilon = (m^2\tau_\varepsilon - \gamma_\varepsilon\tau_\varepsilon^{-1}\theta_\varepsilon)\,d\tau_\varepsilon$$

whence the statement follows since the state A_ε is supersonic and hence $m^2\tau_\varepsilon^2 \geq \gamma_\varepsilon\theta_\varepsilon$.

then is that the curve $\mathcal{C}$ remains in the cell

$$\tau_1 \leq \tau \leq \tau_\varepsilon,\ \theta_\varepsilon \leq \theta \leq \theta_1,\ 0 \leq \varepsilon \leq 1 \quad .$$

This follows from the fact that the field vector at the boundary of this cell points into its interior except on $\varepsilon = 0$.

This statement implies that the curve $\mathcal{C}$ never ends up at the point B_0, since B_0 is evidently not contained in the cell just described. In other words, strong deflagrations are impossible.

Let us denote the points at which the curve $\mathcal{C}$ enters either the surface $\varepsilon = 0$ or the surface $\theta = \theta_s$ as "terminal points" $T_{\mathcal{C}}$. They form a "terminal line" $\mathcal{T}$ which connects the point $\tau = \tau_1$, $\theta = \theta_1$, $\varepsilon = 0$ (for infinite S) with the point A^s (for $S = 0$).

The terminal point $T_{\mathcal{C}}$ depends continuously1) on the reaction rate S. Therefore, if we let S vary from ∞ to 0, the terminal point will move continuously along the terminal line from the plane $\varepsilon = 0$ into the surface $\theta = \theta_s$. Consequently there is a particular value S of S_∞ for which the terminal point lies on the intersection of the plane $\varepsilon = 0$ and the surface $\theta = \theta_s$. We then speak of the "extreme" situation and the "extreme" terminal point $T^\bullet$. Otherwise, if the terminal point lies on the surface $\theta = \theta_s$, we speak of a "normal" situation, if it lies on $\varepsilon = 0$, of an "abnormal" one.

In the extreme situation a weak detonation exists; for, since $\theta = \theta_s$ at the extreme terminal point, the solution curve starting at this point remains on the surface $\varepsilon = 0$. That this solution curve ends up at A_0 follows from the fact that the field has an attractive singularity at A_0 and that the terminal point $T^\bullet = (\tau^\bullet, \theta^\bullet)$ lies in the cell $\tau_1 \leq \tau^\bullet \leq \tau_0$, $p_0 \leq p^\bullet \leq p_1$ and hence belongs to those points that are attracted by A_0. It is clear

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1) This follows immediately from $d\theta/dx \neq 0$ on $\theta = \theta_s$, $\varepsilon > 0$ and $d\varepsilon/dx \neq 0$ on $\varepsilon = 0$, $\theta > \theta_s$; the continuity at $\theta = \theta_s$, $\varepsilon = 0$ can be shown by a more refined consideration.

that a solution curve can reach A_0 only if its terminal point lies on $\varepsilon = 0$ and $\Theta = \Theta_s$. Hence, a weak detonation exists only in the extreme situation, i.e. if the reaction rate S assumes a particular high value S^*.

The discussion of the terminal line $\mathcal{T}$ will also be useful for the investigation of strong detonations. Before we enter the discussion of strong detonations and weak deflagrations we must investigate the possible continuations of solution curves after they have entered the region $\Theta \leq \Theta_s$.

In the region $\Theta \leq \Theta_s$ the actual vector field agrees with the projected vector field. Suppose the point $B_\varepsilon = (\tau_\varepsilon, \Theta_\varepsilon, \varepsilon)$ on the curve $\mathcal{B}$ lies below $\Theta = \Theta_s$, i.e. suppose $\Theta_\varepsilon < \Theta_s$. Then the vector field has a saddle singularity at B_ε, (see p.31). Consequently, two solution curves, $\mathcal{D}_\varepsilon^+$ and $\mathcal{D}_\varepsilon^-$, leave B_ε (see Fig.3); and two solution curves, $\mathcal{F}_\varepsilon^+$ and $\mathcal{F}_\varepsilon^-$, enter B_ε; (the curves with $\Theta > \Theta_\varepsilon$ are $\mathcal{D}_\varepsilon^+$ and $\mathcal{D}_\varepsilon^-$, the one with $\Theta < \Theta_\varepsilon$ are $\mathcal{D}_\varepsilon^-$ and $\mathcal{F}_\varepsilon^-$). We see from the vector field (Fig. 3 and Fig. 5) that $\mathcal{D}_\varepsilon^-$ ends up at the point A_ε on $\mathcal{A}$.

A solution curve $\mathcal{S}$ can enter the region $\Theta \leq \Theta_s$ only at a point where $d\Theta/dx \leq 0$, hence only on the section $\mathcal{L}$ of the surface $\Theta = \Theta_s$ cut out by the surface $\mathcal{E}$ (see p.30). The intersection of $\mathcal{L}$ with a plane $\varepsilon = \text{const.}$ will be denoted by $\mathcal{L}_\varepsilon$, (see Fig. 3 and 5). We consider the continuation of the solution curve $\mathcal{S}$ after its entry into $\Theta \leq \Theta_s$ on the segment $\mathcal{L}_\varepsilon$. There are two cases. Either, the point $B_\varepsilon = (\tau_\varepsilon, \Theta_\varepsilon, \varepsilon)$ lies above the plane $\Theta = \Theta_s$, i.e. $\Theta_\varepsilon > \Theta_s$. Then the continuation of $\mathcal{S}$ from $\mathcal{L}_\varepsilon$ on, ends up in the point A_ε, as seen from the vector field (Fig. 3). Or, the point B_ε lies in the region $\Theta \leq \Theta_s$ (see Fig. 5). Then the curve $\mathcal{F}_\varepsilon^+$ entering B_ε with decreasing Θ intersects the segment $\mathcal{L}_\varepsilon$ in a point G_ε. If $\mathcal{S}$ enters $\mathcal{L}_\varepsilon$ on one side of G_ε (on the side with larger τ), its continuation ends up at A_ε as before. If $\mathcal{S}$ enters $\mathcal{L}_\varepsilon$ on the other side its continuation ends up on $\tau = 0$ unless it has left the region $\Theta \leq \Theta_s$ before reaching $\tau = 0$.

If $\mathcal{S}$ enters $\mathcal{L}_\varepsilon$ at G_ε the continuation of $\mathcal{S}$ leads along $\mathcal{F}_\varepsilon$ to B_ε and from there on $\mathcal{S}$ can be either continued along $\mathcal{D}_\varepsilon^-$ up to A_ε or along $\mathcal{D}_\varepsilon^+$ up to $\tau = 0$ unless $\mathcal{D}_\varepsilon^+$ leaves $\theta \leq \theta_s$ before reaching $\tau = 0$.

We now enter the discussion of *strong detonations*. Strong and Chapman-Jouguet detonations imply subsonic or sonic flow in the burnt gas at $x = \infty$. Hence case (B_1) obtains, or the state (1) corresponds to a point B_1. Consequently, according to the statements made earlier, (see Section 3, p. 19) there is a two-parametric set of solutions regular at $x = \infty$. Hence there is a one-parametric set of solution curves $\mathcal{D}$ leaving the point B_1. We want to show that among the curves $\mathcal{D}$ there is a one $\mathcal{D}^*$, which ends up at A_0, and thus represents a strong (or Chapman-Jouguet) detonation.

The set of curves $\mathcal{D}$ is limited by two curves remaining on the plane $\varepsilon = 1$. One of these two curves, $\mathcal{D}_1^+$, leads to larger values of θ, and ends up on the plane $\tau = 0$ at a point H_1 (see Fig. 2). The other curve, $\mathcal{D}_1^-$, leads to smaller values of θ and ends up in the point A_1; it represents the possible shock transition from state A_1 to state B_1. The set of curves $\mathcal{D}$ may be characterized by a parameter β, which for $\beta = 0$ yields $\mathcal{D}_1^+$ and for $\beta = 1$ yields $\mathcal{D}_1^-$.

On the basis of the assumption made earlier (p.32) that the curve $\mathcal{B}$ lies above the plane $\theta = \theta_s$ we see from the remarks made before that all curves $\mathcal{D}$ that enter the plane $\theta = \theta_s$ end up on $\mathcal{A}$; none therefore meet $\mathcal{B}$ below $\theta = \theta_s$ or end up on $\theta = 0$. Therefore the curves $\mathcal{D}$ end up either on $\tau = 0$, $\varepsilon = 0$, or on $\mathcal{A}$. The so defined end points will be called "ultimate" points and denoted by $U_{\mathcal{D}}(S)$ or $U_\beta(S)$.

We investigate whether or not the point U_β depends continuously on the parameter β. The continuity of U_β could be interrupted only in three cases. The first case would be that U_β were the ultimate point of a curve $\mathcal{D}$ which passes through a saddle singularity of the differential equation. This possibility is excluded; for there is no saddle singularity except on $\varepsilon = 1$ since $\mathcal{B}$ was assumed to lie above $\theta = \theta_s$. The second case would be that $d\tau/dx = 0$ at a point U_β on $\tau = 0$; this is excluded for $\theta > 0$ as seen from the differential equation (1). The third case would be that $d\varepsilon/dx = 0$ at a point U_β on $\varepsilon = 0$. This case can arise at points on $\varepsilon = 0$ with $\theta = \theta_s$.

Let β_* be a value of β such that the coordinates ε and θ of U_β approach 0 and θ_s respectively as $\beta \uparrow \beta_*$ (i.e. β approaches β_* from below). A more detailed investigation would show that then $\mathcal{D}^* = \mathcal{D}_{\beta_*}$ ends up at a point $U^* = U_{\beta_*}$ with $\varepsilon = 0$ and $\theta = \theta_s$.

If, for values of β somewhat greater than β_*, the curve $\mathcal{D}_\beta$ ends up on $\varepsilon = 0$ with $\theta > \theta_s$, the point U_β is continuous at β_*. If, however, such a curve $\mathcal{D}_\beta$ does not reach $\varepsilon = 0$ it will meet $\theta = \theta_s$ for a value $\varepsilon > 0$ and end up on it. Thus $U_\beta = A_\varepsilon$ for such values of β, and as $\beta \downarrow \beta^*$ (i.e. as β approaches β^* from above), $U_\beta \rightarrow A_0$. Thus U_β is not continuous at $\beta = \beta^*_*$.

These considerations make it evident that the ultimate points U_β vary continuously from the position $U_0 = H_1$ on, until either β reaches a value β_* for which U^* is on $\varepsilon = 0$, $\theta = \theta_s$ or until for $\beta = 1$ a point U_1 on $\varepsilon = 0$ with $\theta > \theta_s$ is reached without passing through such a point U_*. We maintain that the latter possibility cannot arise in the normal situation $S < S^0$.

To this end we investigate the curves $\mathcal{D}$ for values of β slightly less than 1. They remain near the curve $\mathcal{D}_1^-$ until they come near to the point A_1; from then on they will remain near the curve $\mathcal{C}$, which leaves the point A_1. In the limit, $\beta \rightarrow 1$, we have a curve $\mathcal{D}$ which coincides with $\mathcal{D}_1^-$ up to the point A_1 and then coincides with the curve $\mathcal{C}$. The ultimate point U_1, therefore, lies on $\varepsilon = 0$ with $\theta < \theta_s$ only if this is the case for the terminal point of $\mathcal{C}$, viz. in the "abnormal" situation. In the normal situation no terminal point on $\varepsilon = 0$ with $\theta > \theta_s$ exists. Consequently, in the normal situation there exists an ultimate point U_* on $\varepsilon = 0$ with $\theta = \theta_s$.

The curve $\mathcal{D} = \mathcal{D}_*$ whose ultimate point is U_* remains on the plane $\varepsilon = 0$ after having passed through U_*, and enters the point A_0. It is evident that the curve $\mathcal{D}_*$ represents a strong detonation. Thus we have established that *in normal situations a strong detonation is possible*. It is not so easily seen whether or not strong detonations are possible in the abnormal case since it is not obvious whether or not there are ultimate points on $\varepsilon = 0$ with $\theta = \theta_s$ from which the continuation leads into A_o.

Suppose the value of the reaction rate S is such that we are in a normal situation but near to the extreme situation. Then the ultimate point U^* is near to the terminal point $T_{\mathcal{C}}$ of the curve $\mathcal{C}$. Hence the curve $\mathcal{D}^*$ ending up at U^* will first lie near to the curve $\mathcal{D}_1^-$ leading from B_1 to A_1 and then near to the curve $\mathcal{C}$ leading from A_1 to $T_{\mathcal{C}}$. Thus we see: in the extreme case, in which the point $T^*_{\mathcal{D}}$ falls on $T_{\mathcal{C}}$, the strong detonation is represented by a curve consisting of the curve $\mathcal{D}_1^-$ in the plane $\varepsilon = 0$ from B_1 to A_1, then by $\mathcal{C}$ leading from A_1 to $T_{\mathcal{C}}$ and finally by a section leading from $T_{\mathcal{C}}$ to A_o. In other words: *in the extreme situation not only a weak detonation exists but also a strong detonation which consists of the weak detonation followed by a shock*. In a normal but nearly extreme situation the strong detonation will be approximately a weak detonation followed by a shock. The extreme situation, however, will occur only for extremely high reaction rates.

Let us consider how a detonation looks in the limiting case when the reaction rate approaches zero; as far as the curves in the $(\tau, \theta, \varepsilon)$-space are concerned this is equivalent to assuming that λ and μ approach zero since $\lambda S_\infty/p_o$ and $\mu S_\infty/p_o$ are the essential dimensionless parameters. The field vectors in this case lie almost in the planes $\varepsilon =$ const. except on the lines $\mathcal{A}$ and $\mathcal{B}$. As was stated earlier, the projection of the vector field in the planes $\varepsilon =$ const. has a saddle singularity at the points B_ε . Hence there are two lines $\mathcal{D}_\varepsilon^+$ and $\mathcal{D}_\varepsilon^-$ depending on ε , which lead out of B_ε . For $\varepsilon = 1$ they coincide with $\mathcal{D}_1^+$ and $\mathcal{D}_1^-$. The curve $\mathcal{D}_\varepsilon^+$ leads to larger values of θ, while $\mathcal{D}_\varepsilon^-$ leads to smaller values of θ. In the limit $S \rightarrow 0$, or, in dimensionless form, $\mu S_\infty / p_o \rightarrow 0$ and $\lambda S_\infty / p_o \rightarrow 0$, the solution curves $\mathcal{D}$ leaving the point B_1 consist of sections of the curve $\mathcal{B}$ followed by the curves $\mathcal{D}_\varepsilon^+$ or $\mathcal{D}_\varepsilon^-$ until these meet the plane $\tau = 0$ or the line $\mathcal{A}$. From this remark it is clear that the ultimate points $U_\beta = U_\beta(0)$ on the plane $\varepsilon = 0$ consist of the curve $\mathcal{D}_o^+$ on $\varepsilon = 0$ from the point H_o on the plane $\tau = 0$ to the point B_o, then of the curve $\mathcal{D}_o^-$ up to the point A_o. It is clear from this description that the curve $\mathcal{D}^*(0)$ consists of the curve $\mathcal{B}$ from B_1 to B_o followed by $\mathcal{D}_o^-$ on $\varepsilon = 0$ up to A_o. In the limit case $\mu S / p_o \rightarrow 0$, $\lambda S / p_o \rightarrow 0$, therefore, the strong detonation consists of a shock followed by a reaction process, as expected.[1]

Finally we are going to show that weak deflagrations exist unless the reaction rate exceeds a certain bound. To this end we should find out whether or not any of the curves $\mathcal{D}$ starting at the point B_1 can end up at the point B_o. The situation differs from that for detonations in that it must now be assumed that $\theta < \theta_s$ at B_o, (see p.32 and Fig. 5). As a consequence the line $\mathcal{U}(S)$ of ultimate points $U_\beta(S)$ is modified for small values of S. For large values of S, the situation is as before. For $S = \infty$, the initial part of the ultimate line $\mathcal{U}(S)$ leads from the point H_1 on $\tau = 0$ straight over to the projection of H_1 on $\varepsilon = 0$. For large values of S, therefore, the ultimate line $\mathcal{U}(S)$ also begins at H_1 and leads on the plane $\tau = 0$ over to the plane $\varepsilon = 0$. From there on U leads on $\varepsilon = 0$ to the point $\mathcal{T}_\beta$ if $\theta > \theta_s$ at A_1, or to a point U^* if $\theta < \theta_s$ at A_1.

For small values of S, however, the situation is quite different. We can no longer assert that the ultimate line leads over from H_1 on the plane $\tau = 0$ to the plane $\varepsilon = 0$. As a matter of fact, for small values of S the ultimate line stops on $\tau = 0$

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[1] If this picture of a detonation is accepted, then v. Neumann's result that no weak detonations exist is implied by the fact that the curve $\mathcal{B}$ connects the point B_o with B_1 and not with A_1.

at a point with $\varepsilon > 0$ and jumps discontinuously over to the line $\mathcal{A}$; the reason being that a curve $\mathcal{D}$ exists which enters the line $\mathcal{B}$ below $\theta = \theta_s$; (this possibility was excluded for detonations, (see pp.36,37). We first consider the case $S = 0$. In that case the curves $\mathcal{D}$ consist of sections of the curve $\mathcal{B}$ followed by sections of the curves $\mathcal{D}_\varepsilon^+$ or $\mathcal{D}_\varepsilon^-$ (see Fig. 4). Since the curve $\mathcal{B}$ now meets the plane $\theta = \theta_s$ before $\varepsilon = 0$ is reached it is clear that none of the curves $\mathcal{D}$ will reach the plane $\varepsilon = 0$.

The ultimate line $\mathcal{U}(0)$ in this case consists of the intersections of the lines $\mathcal{D}_\varepsilon^+$ with $\tau = 0$ from H_1 on up to a value $\varepsilon = \varepsilon_s$ for which $\mathcal{B}$ intersects $\theta = \theta_s$, from there on of the part of the curve $\mathcal{A}$ with $\varepsilon > \varepsilon_s$. The ultimate line thus suffers a discontinuity. Evidently we have $\varepsilon \leq \varepsilon_s$ on the line $\mathcal{U}(0)$. This confirms the statement that $\mathcal{U}(0)$ does not reach the plane $\varepsilon = 0$.

It is now clear that for sufficiently small values of S the ultimate line $\mathcal{U}(S)$ will also not reach the plane $\varepsilon = 0$. As for $S = 0$, the ultimate line will consist of one part on the plane $\tau = 0$ and another part which is a section of the curve . The values of the parameter β referring to these two parts are separated by a value $\hat{\beta}_0(S)$ such that the solution curve $\mathcal{D}_{\hat{\beta}_0}$ enters the point $G_{\hat{\varepsilon}}$ for a certain value $\hat{\varepsilon}(S)$ of ε and then enters the point $B_{\hat{\varepsilon}}$. (We recall that G_ε is the point at which the solution curve $\mathcal{F}_\varepsilon^+$ through B_ε intersects the plane $\theta = \theta_s$, see p.35.) For sufficiently large values of S no such value $\hat{\varepsilon}$ of ε exists since then the ultimate line remains above $\theta = \theta_s$ until it ends at $\mathcal{T}_\phi$ or U^*. Therefore, there is a largest value S^o of S for which a value $\hat{\varepsilon}$ exists. It is then seen that this value is $\hat{\varepsilon} = 0$. Consequently, there is a value β^o of β such that the curve $\mathcal{D}^o = \mathcal{D}_{\beta^o}$ for $S = S^o$ meets the plane $\varepsilon = 0$ at the point G_0 and ends up at the point B_0. This curve $\mathcal{D}^o$ then represents a weak deflagration. Thus we have shown that for every value of the flux m and for an appropriate reaction rate a weak deflagration exists.

The argument presented holds just as well if the points A_1 and B_1 coalesce so that the flow corresponding to this point is sonic. Thus we see that *for an appropriate reaction rate Chapman-Jouguet deflagrations are possible*.

In the limiting case where m and S_∞ approach zero in such a way that $s = S_\infty/m^2$ approaches a finite value, a deflagration is always possible for an appropriate value of S_∞/m^2, as was shown in Section 3. In this limiting case $d\theta = 0$ and $d\varepsilon = 0$ for the vector field except on the plane $\theta = P\tau$, on which the vector field is given by $(\tilde{2})$, $(\tilde{3})$; (see p.25). The points B_0 and B_1 lie on this plane $\theta = p\tau$. The line $\mathcal{D}_1^+$ is the line $\theta = \theta_1$ on $\varepsilon = 1$ with decreasing τ. The line $\mathcal{F}_0^+$ is the line $\theta = P\tau$ on $\varepsilon = 0$ with increasing τ. The point G_0 is then the intersection of $\theta = P\tau$ with $\theta = \theta_s$. As is easily seen there is only one line $\mathcal{D}$ on the plane $\theta = P\tau$ and this line meets the point G_0 only for a special value s_0 of $s = S/m^2$.

Suppose we let m increase holding the initial state (τ_0, θ_0) fixed. Let S(m) be the value of S for which a deflagration exists. We have not proved that S depends continuously on m, but we can be sure that a continuous curve of points (m,S) in a (m,S)-plane exists representing pairs of values of m and S for which deflagrations are possible. Eventually the flux m will reach a value m_C for which the points A_1 and B_1 coalesce and a Chapman-Jouguet situation arises. Let S_C be the corresponding value of the reaction rate S. Then we can at least say that *for every value of the reaction rate $S \leq S_C$ deflagrations are possible with an appropriate value of the flux m*.

APPENDIX I

On The Assumption About the Discontinuous Character Of The Reaction Process

The considerations of this report rest on the "basic" assumption (see p. 3) that the reaction process may be considered approximately a sharp discontinuity; more specifically, that, firstly, the rates of change of the pertinent quantities in the field of flow outside of the reaction zone are negligibly small when compared to the rates of change of the same quantities inside the reaction zone and, secondly, that the rate of change of the width of the reaction zone is small when compared with the average speed with which the gases cross the reaction zone. It was further assumed (p.19) that the flow, when observed from a frame moving with the instantaneous velocity of the reaction front, is steady in the neighborhood of the reaction front at the time considered.

We first want to show that this latter assumption is consistent with the assumption of the discontinuous character of the reaction. Suppose we define the velocity $\dot{x}$ of a border of the reaction zone by $u_t + \dot{x}u_x = 0$, and suppose we choose the velocity of our frame such that $x = 0$ at one point inside the reaction zone. Then the assumption that the rate of change of the width of the reaction zone is small compared with the average gas velocity in the zone can then be formulated as $|\dot{x}| << u$ everywhere in the zone. Consequently, $|u_t| << |uu_x|$ everywhere in the zone. The term u_t, can, therefore, be omitted from the differential equation which expresses the fact that the acceleration $u_t + uu_x$ equals the total applied force per unit mass. For similar reasons one can omit the terms τ_t, θ_t, and ε_t from the differential equations expressing the balance of mass flow, energy, and chemical reaction. In other words, to the degree of accuracy implied by our basic assumption, the equations characterizing non-steady flow reduce to the equations $(1)'$, $(2)'$, $(3)'$ in addition to $m = \text{const.}$ Thus our assumption of "local steadiness" is in agreement with our "basic" assumption.

Secondly we want to mention that frequently reaction flow processes occur in which our basic assumption is not satisfied. Detonations, consisting of a chemical reaction process initiated by a shock, are frequently followed by rarefaction waves. It is clear that this rarefaction wave interferes with the reaction process, but the interference can be ignored if our basic assumption is satisfied and the changes which the rarefaction wave produces in a section of the width of the reaction zone are insignificant. If, however, the reaction zone is so wide that this interference can no longer be ignored, then pressure and temperature in the reaction zone are diminished and the strength of the initiating shock is reduced. In particular, the speed of the detonation wave is then less than that calculated without interference and could thus be less than that of a Chapman-Jouguet detonation. If the interaction is strong the detonation may eventually cease.

The occurence of a lower detonation limit may be explained in this way, since the reaction rate is low, and hence the reaction zone is wide, if the concentration of the combustible component in the unburnt explosive mixture is low. (See Wendlandt [13]).

Spherical detonation waves maintaining the Chapman-Jouguet condition are possible inasmuch as the detonation process can be considered a discontinuity, as Taylor has shown [14]. The rarefaction wave following the detonation front begins, however, with an infinite rate of change of the significant quantities, (see [14]). Consequently, this rarefaction wave always interferes with the detonation wave noticeably and diminishes its strength and speed. It can thus be understood why the speed of spherical detonation waves is less than required by the Chapman-Jouguet hypothesis. Calculations of such spherical detonation waves with sub-Chapman-Jouguet speed were carried out by Eyring and his collaborators [6], [7] .

The gradual building up of a detonation wave ignited at the closed end of a tube may also be explained as due to the interference of a rarefaction wave with the reaction process. The condition that the flow velocity vanish at the closed end requires that a simple rarefaction wave follow the detonation wave. This rarefaction wave, when it begins, involves an infinite drop of pressure, temperature and velocity; thus a noticeable interference is clearly indicated. (For numerical calculations of the gradual building up of a detonation see [7]).

As regards deflagration processes it would seem probable that combustion processes occur in which the width of the reaction zone widens noticeably. Otherwise it would seem impossible to explain how a flame could ever overtake a shock front preceding it. Such combustion processes would then be analogous to rarefaction waves and not to shock discontinuities. No theoretical treatment of such processes seems to exist.

These remarks are intended to show that the frequently observed deviations from the predictions of the discontinuity theory are not due to the unsteadiness of the process as such but rather to the occurrence of a relatively wide reaction zone which permits the interference of the outside flow with the reaction process.

APPENDIX II

It was shown in the text that for an "excessively" high reaction rate $S = S(p,\theta)$ a weak detonation occurs instead of the Chapman-Jouguet detonation (see p. 38). It is of interest to know how high a reaction rate must be in order to be "excessive" in this sense. The excessive cases are separated from the regular ones by "maximal" cases in which a Chapman-Jouguet detonation is just possible, while such a detonation is impossible for a reaction rate higher than a maximal one. We shall present some such maximal reaction rates numerically. From these results it will appear that for maximal reaction rates the transition zone becomes extremely small, of the order of magnitude of one mean free path, if viscosity and heat conduction are those of air at 300°K and atmospheric pressure. Under these circumstances the notions of viscosity and heat conduction in the transition zone become meaningless. If, however, viscosity and heat conduction are ten times as large as for atmospheric air at 300°K, excessive reaction rates may well be possible. For example, S would then be excessive if it vanishes up to 900°K and equals 16.10^{10} $\sec^{-1}$ or more for higher temperatures. The width of the transition zone would then be about ten times as long as a mean free path.

We assume that unburnt and burnt gas are polytropic with exponents $\gamma_0 = 1.4$ and $\gamma = 1.2$. For the mixture consisting of the fraction ε of burnt gas and $1-\varepsilon$ of unburnt gas we define γ by

$$\frac{1}{\gamma - 1} = \frac{1 - \varepsilon}{\gamma_0 - 1} + \frac{\varepsilon}{\gamma_1 - 1} \quad .$$

Then we have for the energy per unit mass of the mixture the expression

$$E^{(\varepsilon)}(\theta) = \frac{\theta}{\gamma - 1} + (1 - \varepsilon)F \quad ,$$

in which the liberated energy per unit mass Γ is assumed to be

$$\Gamma = 32.5\ \Theta_o$$

which corresponds to a value of 665 cal/gm if the initial temperature is $M_o\Theta_o/R_o = 300^\circ K$ and the molecular weight of the unburnt gas is $M_o = 29$.

About the heat conductivity λ and viscosity μ we have made the assumption

$$\frac{\lambda}{\mu} = \frac{\gamma}{\gamma - 1}$$

which was proposed by Becker [4]. We shall in particular consider as reference value for μ the value

$$\mu_o = 2\cdot 44\cdot 10^{-4}\text{gm/cm sec} .$$

with $\gamma = \gamma_o = 1.4$, the corresponding value of λ is then

$$\lambda_o = 8\cdot 54\cdot 10^{-4}\text{gm/cm sec.}$$

We recall that the customary coefficients of viscosity and heat conductivity are $\frac{4}{3}\mu$, and $R\lambda$ in our notation; (see footnote 3 on p.12).

The reaction rate S was assumed to be zero up to a safety temperature $\Theta = \Theta_s$; for $\Theta > \Theta_s$ we have assumed

$$\mu S = \text{const.} ;$$

thus, if μ is independent of temperature and pressure the same is then assumed of the reaction rate for $\Theta > \Theta_o$. This assumption is rather unrealistic because both the reaction rate and the viscosity will increase with the pressure; but this assumption should be sufficient to given information about the order of magnitude of maximal reaction rates. In Fig. 6 we have plotted such maximal reaction rates, or rather the values $\frac{\mu}{\mu_o} S$, in which μ_o is the reference viscosity given above. For a safety temperature of $900^\circ K$ or $\Theta_s = 3\Theta_o$, for example, we find as maximal value

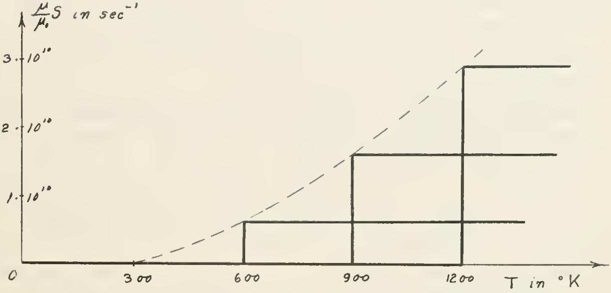

Fig. 6

Maximal reaction rates S as functions of the temperature T.

(If the reaction rate exceeds a maximal one, a Chapman-Jouguet detonation is not possible. μ/μ_0 is the ratio of actual viscosity to that for atmospheric air at room temperature.)

of the reaction rate $S = 16\cdot10^9 \frac{\mu_0}{\mu}$ sec^{-1} for $\Theta > \Theta_s$. The velocity v_0 with which the detonation wave travels into the unburnt gas at rest, solely determined by the Chapman-Jouguet condition, equals $v_0 = 15\cdot7$ m sec^{-1}. The width of the reaction zone is roughly given by

$$\delta = v_0 S^{-1} \quad .$$

In the case $\Theta_s = 3\Theta_0$, $S = 16\cdot10^9 \frac{\mu_0}{\mu}$ sec^{-1}, we therefore have

$$\delta = 98\cdot10^{-7} \frac{\mu}{\mu_0} \text{ cm} ,$$

a length which for $\mu = \mu_0$ would be about equal to one free mean path in air.

To determine maximal reaction rates we observe that the Chapman-Jouguet condition cannot be satisfied if it would lead to a situation called "abnormal" in Sec. 5,p.34. In abnormal situations, the curve $\mathcal{C}$ starting at the point $\mathcal{A}_1$, ends up on the plane $\varepsilon = 0$ with a value $\theta > \theta_s$.

A maximal situation, in which the Chapman-Jouguet condition can just be satisfied, therefore corresponds to what was called an "extreme" situation, in which the curve $\mathcal{C}$ ends up on $\varepsilon = 0$ just with $\theta = \theta_s$. To obtain a maximal reaction rate we then proceed as follows. To a given initial state $(\tau_o, p_o \theta_o)$ corresponding to the point $\mathcal{A}_o$, we determine the end state (τ_1, p_1, θ_1) from the Chapman-Jouguet condition. The flux m is then also determined. We now assume any value for the reaction rate S, or rather for μS and determine the curve $\mathcal{C}$. The value of θ with which $\mathcal{C}$ ends upon $\varepsilon = 0$ is then taken as safety temperature θ_s. We finally select those values for the reaction rate S for which the safety temperature turns out to be between 600°K and 900°K.

The curve $\mathcal{C}$ was characterized as the graph of that solution of the differential equation which leaves the point $\mathcal{A}_1$ with decreasing x. All other solution curves entering $\mathcal{A}_1$ lie on $\varepsilon = 1$. Consequently, $\mathcal{C}$ can also be characterized as the only solution curve leaving the point $\mathcal{A}_1$ without $d\varepsilon = 0$. Hence ε can be introduced as parameter. The differential equations then become, after introducing $t = m^2 \tau$.

$$(1-\varepsilon)\mu S \frac{dt}{d\varepsilon} = t(p + t - p_1 - t_1),$$

$$(1-\varepsilon)\gamma\mu S \frac{dpt}{d\varepsilon} = t[pt - \frac{\gamma-1}{2} t^2 + (\gamma-1)tt_1 + (\gamma-1)(1-\varepsilon)fp_1t_1 - p_1t_1 - \frac{\gamma-1}{2}t_1^2].$$

The desired solution $t = t(\varepsilon)$, $p = p(\varepsilon)$ is then the one that assumes the values (t_1, p_1) for $\varepsilon = 1$ and permits expansion with respect to powers of $(1-\varepsilon)$. It is easily obtained from this power series for small values of $(1-\varepsilon)$ and by finite differences for larger values of $1 - \varepsilon$ up to $\varepsilon = 0$.

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